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A new global analytical *ab initio* potential energy surface for the $\text{C}^+(\text{}^2\text{P}) + \text{SH}(\text{X } ^2\Pi)$ reaction

Supporting Information

Lulu Zhang^{1*}, Juan Zhao¹, Dong Liu¹, Wei Wang¹, Daguang Yue¹, Yuzhi Song²,
Qingtian Meng^{2†}

¹School of Science, Shandong Jiaotong University, 250357, Jinan, China

²School of Physics and Electronics, Shandong Normal University, 250358, Jinan, China

* E-mail address: zhanglulu@sdjtu.edu.cn.

† E-mail address: qtmeng@sdu.edu.cn.

Table S1: Fitted parameters of two-body energy term in Eq. (5).

	SH($X^2\Pi$)	CH ⁺ ($a^3\Pi$)
a_0	0.11983944E+02	0.68737672E+01
a_1	-0.42969632E-01	-0.35917843E-01
a_2	0.19288396E+01	0.80198027E+00
a_3	-0.49108817E+02	-0.22760281E+02
a_4	0.63175003E+03	0.24916362E+03
a_5	-0.50970769E+04	-0.18698656E+04
a_6	0.25181313E+05	0.95227039E+04
a_7	-0.78638086E+05	-0.32387824E+05
a_8	0.15689835E+06	0.72034443E+05
a_9	-0.19463422E+06	-0.10054410E+06
a_{10}	0.13707752E+06	0.79987728E+05
a_{11}	-0.41945778E+05	-0.27702082E+05
β_1	1.7040	2.1090
β_2	0.6810	0.7000

Table S2: Fitted parameters of three-body energy term in Eqs. (6) and (7).

a_1	-0.14463219E+02	a_{101}	0.22199425E+04	a_{201}	0.21786267E+07
a_2	0.72673467E+03	a_{102}	0.61966929E+04	a_{202}	0.26595182E+07
a_3	-0.90944544E+04	a_{103}	-0.13290449E+06	a_{203}	-0.25852346E+06
a_4	0.56469738E+05	a_{104}	0.58239441E+06	a_{204}	-0.19049923E+07
a_5	-0.21017664E+06	a_{105}	-0.97129609E+06	a_{205}	0.71250735E+04
a_6	0.49825547E+06	a_{106}	0.22806366E+06	a_{206}	-0.14001067E+06
a_7	-0.74719575E+06	a_{107}	0.56385180E+06	a_{207}	0.19965539E+06
a_8	0.65075812E+06	a_{108}	0.10012545E+04	a_{208}	-0.91041528E+06
a_9	-0.24910876E+06	a_{109}	-0.25101212E+04	a_{209}	0.83616753E+06
a_{10}	-0.13008105E+03	a_{110}	0.34659253E+04	a_{210}	-0.47022940E+06
a_{11}	-0.11869486E+04	a_{111}	0.82035611E+05	a_{211}	-0.45520170E+05
a_{12}	0.35549108E+05	a_{112}	-0.77115375E+05	a_{212}	0.17615173E+06
a_{13}	-0.23600431E+06	a_{113}	-0.60513890E+06	a_{213}	-0.47836732E+06
a_{14}	0.77095966E+06	a_{114}	0.10626809E+07	a_{214}	-0.14919018E+07
a_{15}	-0.13689402E+07	a_{115}	0.31548136E+06	a_{215}	-0.69189655E+06
a_{16}	0.12025313E+07	a_{116}	-0.51998748E+04	a_{216}	0.34954718E+06
a_{17}	-0.37405423E+06	a_{117}	0.28850374E+05	a_{217}	0.11133757E+07
a_{18}	0.57540605E+03	a_{118}	-0.15658893E+06	a_{218}	0.19638631E+07
a_{19}	-0.15706871E+05	a_{119}	0.16860525E+05	a_{219}	0.14423705E+07
a_{20}	0.96318946E+04	a_{120}	0.53027131E+06	a_{220}	-0.55260405E+06
a_{21}	0.24288442E+06	a_{121}	0.78281019E+06	a_{221}	-0.69722910E+06
a_{22}	-0.89203067E+06	a_{122}	-0.25498388E+07	a_{222}	-0.41311654E+06
a_{23}	0.14390802E+07	a_{123}	0.10541697E+05	a_{223}	0.13466755E+06
a_{24}	-0.85070517E+06	a_{124}	-0.32080820E+05	a_{224}	0.81486714E+06
a_{25}	0.84959797E+04	a_{125}	0.35079375E+06	a_{225}	0.19429225E+06
a_{26}	0.62311999E+05	a_{126}	-0.77463380E+06	a_{226}	0.37133260E+06
a_{27}	-0.22698640E+06	a_{127}	-0.97013647E+06	a_{227}	0.42915614E+05
a_{28}	0.14128531E+06	a_{128}	0.98950335E+06	a_{228}	0.13623743E+07
a_{29}	0.15631848E+05	a_{129}	-0.40073685E+05	a_{229}	-0.15796762E+04
a_{30}	-0.21795496E+06	a_{130}	-0.99891413E+05	a_{230}	0.33163800E+04
a_{31}	-0.70832047E+05	a_{131}	0.44010749E+06	a_{231}	-0.10314982E+07
a_{32}	-0.65458740E+05	a_{132}	0.20671757E+07	a_{232}	0.24478723E+06
a_{33}	0.43386084E+06	a_{133}	0.10371668E+06	a_{233}	0.57722945E+06
a_{34}	-0.17753348E+06	a_{134}	0.15171000E+06	a_{234}	-0.43269619E+06
a_{35}	0.18404593E+06	a_{135}	-0.14926106E+06	a_{235}	-0.14478191E+07
a_{36}	0.23364138E+06	a_{136}	-0.24456138E+07	a_{236}	-0.11710827E+07
a_{37}	-0.69722818E+05	a_{137}	-0.19169831E+07	a_{237}	0.59533047E+06
a_{38}	-0.43225772E+06	a_{138}	-0.24128058E+06	a_{238}	-0.32847569E+06
a_{39}	-0.39026296E+05	a_{139}	0.11768747E+07	a_{239}	-0.24061002E+06
a_{40}	-0.40465567E+06	a_{140}	0.22458383E+07	a_{240}	-0.51464417E+06
a_{41}	0.21884032E+06	a_{141}	0.12861586E+06	a_{241}	-0.62984722E+06
a_{42}	0.21765676E+06	a_{142}	-0.11724245E+07	a_{242}	-0.96567331E+06
a_{43}	0.36492704E+06	a_{143}	0.23182259E+04	a_{243}	0.16423105E+06
a_{44}	-0.14822117E+06	a_{144}	-0.54801826E+03	a_{244}	0.19607876E+07
a_{45}	-0.13535607E+06	a_{145}	0.39146305E+04	a_{245}	0.44009978E+05
a_{46}	0.35570499E+02	a_{146}	-0.51177095E+05	a_{246}	0.28135366E+06
a_{47}	-0.24886169E+03	a_{147}	0.20665108E+06	a_{247}	0.12715397E+07
a_{48}	-0.25156350E+04	a_{148}	-0.73187059E+06	a_{248}	-0.20807525E+06
a_{49}	0.51526408E+05	a_{149}	0.19922083E+07	a_{249}	0.32276164E+06
a_{50}	-0.34792365E+06	a_{150}	-0.20588068E+07	a_{250}	0.65167933E+06

a_{51}	0.12124776E+07	a_{151}	-0.69820891E+04	a_{251}	-0.32120152E+06
a_{52}	-0.23306802E+07	a_{152}	-0.26028611E+04	a_{252}	-0.15210083E+07
a_{53}	0.23321936E+07	a_{153}	0.18918611E+05	a_{253}	-0.71568795E+05
a_{54}	-0.96150754E+06	a_{154}	-0.25782534E+06	a_{254}	-0.19902081E+05
a_{55}	-0.61934771E+02	a_{155}	0.42259470E+06	a_{255}	0.20617875E+06
a_{56}	0.45392731E+03	a_{156}	-0.12608808E+07	β_{SH}	0.810
a_{57}	-0.81476055E+03	a_{157}	0.49588936E+06	β_{CS}	0.630
a_{58}	-0.28246490E+05	a_{158}	0.37239244E+05	β_{CH}	0.890
a_{59}	0.22764263E+06	a_{159}	-0.71433165E+05		
a_{60}	-0.65423586E+06	a_{160}	0.34302412E+06		
a_{61}	0.55068275E+06	a_{161}	0.37274609E+06		
a_{62}	0.93161894E+06	a_{162}	-0.90148093E+05		
a_{63}	-0.13011878E+07	a_{163}	0.20154584E+07		
a_{64}	0.36092119E+03	a_{164}	-0.40248886E+05		
a_{65}	-0.32902640E+04	a_{165}	0.23332063E+06		
a_{66}	0.32405474E+05	a_{166}	-0.17216711E+07		
a_{67}	-0.11687705E+06	a_{167}	-0.17162625E+07		
a_{68}	-0.21770337E+06	a_{168}	-0.16815087E+07		
a_{69}	0.17082686E+07	a_{169}	-0.19981402E+05		
a_{70}	-0.37020232E+07	a_{170}	0.55727032E+06		
a_{71}	0.16599199E+07	a_{171}	0.44786525E+07		
a_{72}	-0.10587840E+04	a_{172}	0.33581305E+07		
a_{73}	-0.15613819E+04	a_{173}	-0.91728491E+05		
a_{74}	-0.43931610E+05	a_{174}	-0.24269741E+07		
a_{75}	0.58025701E+06	a_{175}	-0.38232146E+07		
a_{76}	-0.89149155E+06	a_{176}	0.30412093E+06		
a_{77}	0.10109931E+07	a_{177}	0.21961574E+07		
a_{78}	0.18943624E+07	a_{178}	-0.17008285E+06		
a_{79}	0.81276294E+03	a_{179}	0.24795400E+05		
a_{80}	0.29724327E+05	a_{180}	-0.79540237E+05		
a_{81}	-0.17015417E+06	a_{181}	0.35617496E+06		
a_{82}	-0.70111122E+06	a_{182}	-0.37930568E+06		
a_{83}	0.13802083E+06	a_{183}	-0.24006884E+06		
a_{84}	-0.25204583E+07	a_{184}	0.86735641E+06		
a_{85}	0.20506233E+05	a_{185}	0.25486374E+05		
a_{86}	-0.43370515E+05	a_{186}	0.19819761E+05		
a_{87}	0.45942190E+06	a_{187}	-0.10321885E+05		
a_{88}	0.77365015E+06	a_{188}	0.91524595E+05		
a_{89}	0.16636266E+07	a_{189}	0.48010511E+06		
a_{90}	-0.11588693E+06	a_{190}	-0.90354590E+06		
a_{91}	0.62845882E+05	a_{191}	-0.15451606E+06		
a_{92}	-0.45599726E+06	a_{192}	-0.17008888E+06		
a_{93}	-0.93537453E+06	a_{193}	0.44870404E+06		
a_{94}	0.26279325E+06	a_{194}	0.16693358E+07		
a_{95}	-0.16738436E+06	a_{195}	0.80636743E+06		
a_{96}	0.26857950E+06	a_{196}	0.21263409E+06		
a_{97}	-0.27648662E+06	a_{197}	-0.82046124E+06		
a_{98}	0.14832938E+06	a_{198}	-0.31364022E+07		
a_{99}	0.11219001E+06	a_{199}	-0.31502478E+07		
a_{100}	-0.39253808E+03	a_{200}	0.96102251E+05		
